

RELATIVISTIC COULOMB INTEGRALS AND ZEILBERGER'S HOLONOMIC SYSTEMS APPROACH. I

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Dedicated to Doron Zeilberger on the occasion of his 60th birthday.

ABSTRACT. With the help of computer algebra we study the diagonal matrix elements $\langle Or^p \rangle$, where $O = \{1, \beta, i\alpha n\beta\}$ are the standard Dirac matrix operators and the angular brackets denote the quantum-mechanical average for the relativistic Coulomb problem. Using Zeilberger's extension of Gosper's algorithm and a variant to it, three-term recurrence relations for each of these expectation values are derived together with some transformation formulas for the corresponding generalized hypergeometric series. In addition, the virial recurrence relations for these integrals are also found and proved algorithmically.

Science is what we understand well enough to explain to a computer. Art is everything else we do.

Donald E. Knuth [22]

1. INTRODUCTION

This work has been initiated by the following email regarding Doron Zeilberger's Z60 conference:

<http://www.math.rutgers.edu/events/Z60/>

Email to Peter Paule from Sergei Suslov [27 Feb 2010]

Subject: Uranium 91+ ion

"...I understand that you are coming to Doron's conference in May and write to you with an unusual suggestion..."

I am attaching two of my recent papers inspired by recent success in checking Quantum Electrodynamics in strong fields [see Refs. [36] and [38] in this paper].

It is a very complicated problem theoretically, and fantastically, enormously complicated (at the level of science fiction!) experimentally, which has been solved - after 20 years of hard work by theorists from Russia (Shabaev + 20 coauthors/students) and experimentalists from Germany.

Experimentally they took a uranium 92 atom, got rid of all but one electrons, and measured the energy shifts due to the quantization of the electromagnetic radiation field!

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Mathematically, among other things, the precise structure of the energy levels of the U 91+ ion requires the evaluation of certain relativistic Coulomb integrals, done, in a final form, in my attached papers ...

Here is the problem:

These integrals have numerous recurrence relations found by physicists on the basis of virial theorems. They are also sums of 3 (linearly dependent) 3F2 series.

Now you can imagine what a mess it is if one tries to derive those relations at the level of hypergeometric series (3 times 3 = 9 functions usually!).

It looks as a perfect job for the G-Z algorithm in a realistic (important) classical problem of relativistic quantum mechanics. It looks as a good birthday present to Doron, if one could have done that. I feel we can do that together.

Looking forward to your answer on my crazy suggestion, BW, Sergei"

The first named author's computer algebra response reported at the Z60 conference is presented in this joint paper.

2. RELATIVISTIC COULOMB INTEGRALS

Recent experimental and theoretical progress has renewed interest in quantum electrodynamics of atomic hydrogenlike systems (see, for example, [3], [10], [11], [13], [14], [17], [32], [34], [35] and the references therein). In the last decade, the two-time Green's function method of deriving formal expressions for the energy shift of a bound-state level of high- Z few-electron systems was developed [32] and numerical calculations of QED effects in heavy ions were performed with an excellent agreement to current experimental data [10], [11], [34]. These advances motivate a detailed study of the expectation values of the Dirac matrix operators multiplied by the powers of the radius between the bound-state relativistic Coulomb wave functions. Special cases appear in calculations of the magnetic dipole hyperfine splitting, the electric quadrupole hyperfine splitting, the anomalous Zeeman effect, and the relativistic recoil corrections in hydrogenlike ions (see, for example, [1], [31], [33], [36] and the references therein). These expectation values can be used in calculations with hydrogenlike wave functions when a high precision is required. For applications of the off-diagonal matrix elements, see [23], [24], [25], [29], [30], and [33].

Two different forms of the radial wave functions F and G are available (see, for example, [19] and [39]). Given a set of parameters $a, \alpha_1, \alpha_2, \beta, \beta_1, \beta_2$, and γ , depending on physical constants ε, κ, μ , and ν , consider

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = a^2 \beta^{3/2} \sqrt{\frac{n!}{\gamma \Gamma(n+2\nu)}} (2a\beta r)^{\nu-1} e^{-a\beta r} \begin{pmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{pmatrix} \begin{pmatrix} L_{n-1}^{2\nu}(2a\beta r) \\ L_n^{2\nu}(2a\beta r) \end{pmatrix} \quad (2.1)$$

where, using the notation from [20], $L_n^\lambda(x)$ stands for the corresponding Laguerre polynomial of order n . Throughout this paper,

$$\begin{aligned} \kappa &= \pm(j+1/2), & \nu &= \sqrt{\kappa^2 - \mu^2}, \\ \mu &= \alpha Z = Ze^2/\hbar c, & a &= \sqrt{1 - \varepsilon^2}, \\ \varepsilon &= E/mc^2, & \beta &= mc/\hbar, \end{aligned} \quad (2.2)$$

and $\gamma = \mu(\kappa - \nu)(\varepsilon\kappa - \nu)$, with the total angular momentum $j = 1/2, 3/2, 5/2$, etc. (see [4], [5], [8], [26], [36], and [39] regarding the relativistic Coulomb problem). The following identities

$$\begin{aligned} \varepsilon\mu &= a(\nu + n), \quad \varepsilon\mu + a\nu = a(n + 2\nu), \quad \varepsilon\mu - a\nu = an, \\ \varepsilon^2\kappa^2 - \nu^2 &= a^2n(n + 2\nu) = \mu^2 - a^2\kappa^2 \end{aligned} \quad (2.3)$$

are useful in the calculation of the matrix elements.

The relativistic Coulomb integrals of the radial functions,

$$A_p = \int_0^\infty r^{p+2} (F^2(r) + G^2(r)) dr, \quad (2.4)$$

$$B_p = \int_0^\infty r^{p+2} (F^2(r) - G^2(r)) dr, \quad (2.5)$$

$$C_p = \int_0^\infty r^{p+2} F(r) G(r) dr, \quad (2.6)$$

have been evaluated in Refs. [36] and [38] for all admissible integer powers p , in terms of linear combinations of special generalized hypergeometric ${}_3F_2$ series related to the Chebyshev polynomials of a discrete variable [18], [19].

Note. We concentrate on the radial integrals since, for problems involving spherical symmetry, one can reduce all expectation values to radial integrals by use of the properties of angular momentum.

Throughout the paper we use the following abbreviated form of the standard notation of the generalized hypergeometric series ${}_3F_2$; see, e.g., [20]:

$${}_3F_2 \left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix} \right) := {}_3F_2 \left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix} ; 1 \right) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k (a_3)_k}{(b_1)_k (b_2)_k k!}, \quad (2.7)$$

where $(a)_k := a(a+1)\dots(a+k-1)$ denotes the Pochhammer symbol.

Analogues of the traditional hypergeometric representations for the integrals are as follows [36]:

$$\begin{aligned} 2\mu(2a\beta)^p \frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)} A_p &= 2p\varepsilon an {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 2 \end{matrix} \right) \\ &+ (\mu + a\kappa) {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right) + (\mu - a\kappa) {}_3F_2 \left(\begin{matrix} -n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right), \end{aligned} \quad (2.8)$$

$$\begin{aligned} 2\mu(2a\beta)^p \frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)} B_p &= 2pan {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 2 \end{matrix} \right) \\ &+ \varepsilon(\mu + a\kappa) {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right) + \varepsilon(\mu - a\kappa) {}_3F_2 \left(\begin{matrix} -n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right), \end{aligned} \quad (2.9)$$

$$\begin{aligned} 4\mu(2a\beta)^p \frac{\Gamma(2\nu+1)}{\Gamma(2\nu+p+1)} C_p \\ = a(\mu + a\kappa) {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right) - a(\mu - a\kappa) {}_3F_2 \left(\begin{matrix} -n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right). \end{aligned} \quad (2.10)$$

The averages of r^p for the relativistic hydrogen atom, namely the integrals A_p , were evaluated in the late 1930s by Davis [6] as a sum of certain three ${}_3F_2$ functions.¹ But it has been realized only recently that these series are, in fact, linearly dependent and related to the Chebyshev polynomials of a discrete variable [36]. The most compact forms in terms of only two linearly independent generalized hypergeometric series are given in Ref. [38].

In addition, the integrals themselves are linearly dependent:

$$(2\kappa + \varepsilon(p+1)) A_p - (2\varepsilon\kappa + p+1) B_p = 4\mu C_p; \quad (2.11)$$

see, for example, [1], [29], [30], and [36]. Thus, eliminating, say C_p , one can deal with A_p and B_p only.

The integrals (2.4)–(2.6) satisfy numerous recurrence relations in p , which provide an effective way of their evaluation for small p . A set of useful recurrence relations between the relativistic matrix elements was derived by Shabaev [30] (see also [1], [7], [29], [33], [36], and [40]) on the basis of a hypervirial theorem:

$$2\kappa A_p - (p+1) B_p = 4\mu C_p + 4\beta\varepsilon C_{p+1}, \quad (2.12)$$

$$2\kappa B_p - (p+1) A_p = 4\beta C_{p+1}, \quad (2.13)$$

$$\mu B_p - (p+1) C_p = \beta (A_{p+1} - \varepsilon B_{p+1}). \quad (2.14)$$

From these relations one can derive (see [1], [30], and [33]) the linear relation (2.11) and the following computationally convenient recurrence formulas (2.15)–(2.18), stated in our notation as

$$\begin{aligned} A_{p+1} = & -(p+1) \frac{4\nu^2\varepsilon + 2\kappa(p+2) + \varepsilon(p+1)(2\kappa\varepsilon + p+2)}{4(1-\varepsilon^2)(p+2)\beta\mu} A_p \\ & + \frac{4\mu^2(p+2) + (p+1)(2\kappa\varepsilon + p+1)(2\kappa\varepsilon + p+2)}{4(1-\varepsilon^2)(p+2)\beta\mu} B_p, \end{aligned} \quad (2.15)$$

$$\begin{aligned} B_{p+1} = & -(p+1) \frac{4\nu^2 + 2\kappa\varepsilon(2p+3) + \varepsilon^2(p+1)(p+2)}{4(1-\varepsilon^2)(p+2)\beta\mu} A_p \\ & + \frac{4\mu^2\varepsilon(p+2) + (p+1)(2\kappa\varepsilon + p+1)(2\kappa + \varepsilon(p+2))}{4(1-\varepsilon^2)(p+2)\beta\mu} B_p \end{aligned} \quad (2.16)$$

and

$$\begin{aligned} A_{p-1} = & \beta \frac{4\mu^2\varepsilon(p+1) + p(2\kappa\varepsilon + p)(2\kappa + \varepsilon(p+1))}{\mu(4\nu^2 - p^2)p} A_p \\ & - \beta \frac{4\mu^2(p+1) + p(2\kappa\varepsilon + p)(2\kappa\varepsilon + p+1)}{\mu(4\nu^2 - p^2)p} B_p, \end{aligned} \quad (2.17)$$

$$\begin{aligned} B_{p-1} = & \beta \frac{4\nu^2 + 2\kappa\varepsilon(2p+1) + \varepsilon^2p(p+1)}{\mu(4\nu^2 - p^2)} A_p \\ & - \beta \frac{4\nu^2\varepsilon + 2\kappa(p+1) + \varepsilon p(2\kappa\varepsilon + p+1)}{\mu(4\nu^2 - p^2)} B_p, \end{aligned} \quad (2.18)$$

respectively.

¹He finishes his article by saying: “In conclusion I wish to thank Professors H. Bateman, P. S. Epstein, W. V. Houston, and J. R. Openheimer for their helpful suggestions.”

Note. (i) These recurrences are complemented by the symmetries of the integrals A_p , B_p , and C_p under the reflections $p \rightarrow -p - 1$ and $p \rightarrow -p - 3$ found in [36]; see also [2]. (ii) These relations were also derived in [37] by a different method using relativistic versions of the Kramers–Pasternack three-term recurrence relations.

3. COMPUTER ALGEBRA AND SOFTWARE

The general algorithmic background of the computer algebra applications in this paper is Zeilberger’s path-breaking holonomic systems paper [41]. The examples given in the following sections restrict to applications: (i) of Zeilberger’s extension [43] of Gosper’s algorithm [9], also called Zeilberger’s “fast algorithm” [42, 22], and (ii) of a variant of it which has been described in the unpublished manuscript [21]. Both of these algorithms have been implemented in the Fast Zeilberger package **zb.m** which is written in *Mathematica* and whose functionality is illustrated below. A very general framework of Zeilberger’s creative telescoping (i), and also of its variant (ii), is provided by Schneider’s extension of Karr’s summation in difference fields [12]; see, for instance, [27, 28] and the references therein.

The Fast Zeilberger Package can be obtained freely from the site

<http://www.risc.jku.at/research/combinat/software/>

after sending a password request to the first named author. Put the package **zb.m** in some directory, e.g., `/home/mydirectory`, open a *Mathematica* session, and read in the package by

```
In[1]:= SetDirectory["/home/ppaule/RISC_Comb_Software_Sep05.dir/fastZeil"];
<<zb.m
```

Fast Zeilberger Package by Peter Paule and Markus Schorn (enhanced by Axel Riese)
- © RISC Linz - V 3.53 (02/22/05)

A *Mathematica* notebook containing a full account of the *Mathematica* sessions described below, together with some additional material, is available at:

<http://hahn.la.asu.edu/~suslov/curres/index.htm>

4. UNMIXED THREE-TERM RECURRENCE RELATIONS

The following relations purely in the A_p and B_p , respectively, have been established in [38]:

$$A_{p+1} = \frac{\mu P(p)}{a^2 \beta (4\mu^2 (p+1) + p(2\varepsilon\kappa + p)(2\varepsilon\kappa + p+1))(p+2)} A_p - \frac{(4\nu^2 - p^2)(4\mu^2 (p+2) + (p+1)(2\varepsilon\kappa + p+1)(2\varepsilon\kappa + p+2))p}{(2a\beta)^2 (4\mu^2 (p+1) + p(2\varepsilon\kappa + p)(2\varepsilon\kappa + p+1))(p+2)} A_{p-1}, \quad (4.1)$$

$$B_{p+1} = \frac{\varepsilon\mu Q(p)}{a^2 \beta (4\nu^2 + 2\varepsilon\kappa(2p+1) + \varepsilon^2 p(p+1))(p+2)} B_p - \frac{(4\nu^2 - p^2)(4\nu^2 + 2\varepsilon\kappa(2p+3) + \varepsilon^2 (p+1)(p+2))(p+1)}{(2a\beta)^2 (4\nu^2 + 2\varepsilon\kappa(2p+1) + \varepsilon^2 p(p+1))(p+2)} B_{p-1}, \quad (4.2)$$

where

$$P(p) = 2\varepsilon p(p+2)(2\varepsilon\kappa+p)(2\varepsilon\kappa+p+1) + \varepsilon [4(\varepsilon^2\kappa^2 - \nu^2) - p(4\varepsilon^2\kappa^2 + p(p+1))] + (2p+1)[4\varepsilon^2\kappa + 2(p+2)(2\varepsilon\mu^2 - \kappa)], \quad (4.3)$$

$$Q(p) = (2p+3)[4\nu^2 + 2\varepsilon\kappa(2p+1) + p(p+1)] - a^2(2p+1)(p+1)(p+2). \quad (4.4)$$

In comparison with other papers (e.g., [1], [2], [29], [30], [36], [37], and the references therein), this approach provides an alternative way of the recursive evaluation of the special values A_p and B_p , when one deals separately with one of these integrals only. The corresponding initial data $A_0 = 1$ and $B_{-1} = a^2\beta/\mu$ can be found in [36].

Note. The derivation in [38] resembles the reduction (uncoupling) of the first order system of differential equations for relativistic radial Coulomb wave functions F and G to the second order differential equations; see, for example, [19] and [39].

With Zeilberger's definite extension [42, 43] of Gosper's algorithm [9] for indefinite hypergeometric summation, the derivation of such recurrences is fully automatic if the input is given as a terminating hypergeometric series (and provided that the input is of computationally feasible size). We illustrate this by a mechanical derivation of the following simple three-term recurrence relation for the integral C_p , not found in [38]:

$$C_{p+1} = \mu(2p+1) \frac{2\kappa + \varepsilon[p(p+1) - 4\kappa^2]}{a^2\beta(p^2 - 4\kappa^2)(p+1)} C_p + p \frac{(p^2 - 4\nu^2)[(p+1)^2 - 4\kappa^2]}{(2a\beta)^2(p^2 - 4\kappa^2)(p+1)} C_{p-1}. \quad (4.5)$$

As input for C_p we take the hypergeometric sum representation from (2.10). We start our *Mathematica* session by reading in the RISC "Fast Zeilberger" package:

```
In[1] := <<zbl.m
```

```
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```

```
In[2] := (a_)k_ := Pochhammer[a,k];
```

$$F1[k_] := \frac{(1-n)_k (-p)_k (p+1)_k}{(2\nu+1)_k (1)_k k!}; \quad F2[k_] := \frac{(-n)_k (-p)_k (p+1)_k}{(2\nu+1)_k (1)_k k!};$$

```
In[3] := FullSimplify[{F1[k]/F1[k], F2[k]/F1[k]}]
```

$$\text{Out}[3] = \{1, -\frac{n}{k-n}\}$$

$$\text{In}[4] := f[k_] := \left(4\mu(2a\beta)^p \frac{\text{Gamma}[2\nu+1]}{\text{Gamma}[2\nu+p+1]}\right)^{-1} * F1[k] * \left(a(\mu+a\kappa) - a(\mu-a\kappa) * \frac{n}{n-k}\right);$$

In[5]:= SuslovRec=Zb[f[k] , k, 0, Infinity, p, 2] // Simplify

Out[5]= {4 a β (−(3+2 p) (−(2+3 p+p²) μ² (n+ν) − 2 a n κ μ (n+2 ν)+
a² κ² (n+ν) (2+4 n²+3 p+p²+8 n ν)) SUM[1+p] +
a (2+p) β (−(1+p)² μ²+a² κ² (4 n²+(1+p)²+8 n ν)) SUM[p+2] ==
(1+p) (1+2 p+p²−4 ν²) (−(2+p)² μ²+a² κ² (4 n²+(2+p)²+8 n ν)) SUM[p]}

Here $C_p = \text{SUM}[p]$. Utilizing two of the identities (2.2)–(2.3) brings Out[5] into the form (4.5). In order to *prove* the correctness of Out[5], just type

In[6]:= Prove[]

and the program generates automatically a pretty print version of a proof in a separate window or file, respectively.

The computerized derivations and proofs of (4.1)–(4.2) are analogous; one finds the details in the corresponding *Mathematica* notebooks on the article's website.

5. RELATED TRANSFORMATIONS OF GENERALIZED HYPERGEOMETRIC SERIES

Several relations between two pairs of the generalized hypergeometric series under consideration are given in [36] and [38]:

$$\begin{aligned}
& {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right) \\
&= \frac{(2\nu+n)(2\nu+p+1)(2\nu+p+2)(2n+p+1)}{4\nu(2\nu+1)(\nu+n)(p+1)} \\
&\quad \times {}_3F_2 \left(\begin{matrix} 1-n, p+2, -p-1 \\ 2\nu+2, 1 \end{matrix} \right) \\
&\quad - \frac{n(4\nu+2n+p+1)}{2(\nu+n)(p+1)} {}_3F_2 \left(\begin{matrix} -n, p+2, -p-1 \\ 2\nu, 1 \end{matrix} \right)
\end{aligned} \tag{5.1}$$

and

$$\begin{aligned}
& {}_3F_2 \left(\begin{matrix} -n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right) \\
&= \frac{n(4\nu+2n-p-1)(2\nu+p+1)(2\nu+p+2)}{4\nu(2\nu+1)(\nu+n)(p+1)} \\
&\quad \times {}_3F_2 \left(\begin{matrix} 1-n, p+2, -p-1 \\ 2\nu+2, 1 \end{matrix} \right) \\
&\quad - \frac{(2\nu+n)(2n-p-1)}{2(\nu+n)(p+1)} {}_3F_2 \left(\begin{matrix} -n, p+2, -p-1 \\ 2\nu, 1 \end{matrix} \right).
\end{aligned} \tag{5.2}$$

In addition,

$$\begin{aligned}
& \frac{p(p+1)}{2\nu+n} {}_3F_2 \left(\begin{matrix} 1-n, p+1, -p \\ 2\nu+1, 2 \end{matrix} \right) \\
&= \frac{(p-2\nu)(2\nu+p+1)}{2(2\nu+1)(\nu+n)} {}_3F_2 \left(\begin{matrix} 1-n, p+1, -p \\ 2\nu+2, 1 \end{matrix} \right) \\
&+ \frac{\nu}{\nu+n} {}_3F_2 \left(\begin{matrix} -n, p+1, -p \\ 2\nu, 1 \end{matrix} \right),
\end{aligned} \tag{5.3}$$

and

$$\begin{aligned}
& \frac{p(p+1)}{n+2\nu} {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 2 \end{matrix} \right) \\
&= {}_3F_2 \left(\begin{matrix} -n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right) - {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right).
\end{aligned} \tag{5.4}$$

These relations are “responsible” for the transformation between two different hypergeometric forms of the relativistic Coulomb integral [36, 38]. The second named author was able to give only the proof of the last relation from the advanced theory of generalized hypergeometric functions.

With the `zb.m` package, one can not only prove but also find such relations, in the literature called also contiguous relations, automatically. We illustrate this by a computer derivation of (5.1).

```
In[1] := <<zb.m
```

```
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```

```
In[2] := (a_)_ := Pochhammer[a,k];    F0[k_] := (1-n)_k (-p)_k (p+1)_k /
(2 ν+1)_k (1)_k k!;
F1[k_] := (1-n)_k (-p-1)_k (p+2)_k / (2 ν+2)_k (1)_k k!; F2[k_] := (-n)_k (-p-1)_k (p+2)_k /
(2 ν)_k (1)_k k!;
```

Our goal is to compute rational function coefficients c_0, c_1, c_2 , free of the summation variable k , such that

$$\sum_{k=0}^{\infty} (c_0 F0[k] + c_1 F1[k] + c_2 F2[k]) = 0.$$

With a parameterized version of Gosper’s algorithm, similar to Zeilberger’s extension of Gosper’s algorithm, we compute such c_i together with a hypergeometric expression g such that for non-negative integer N :

$$\sum_{k=0}^N \left(F0[k] \left(c_0 + c_1 \frac{F1[k]}{F0[k]} + c_2 \frac{F2[k]}{F0[k]} \right) \right) = g[N].$$

This is accomplished using the option `Parameterized`; finally we send N to infinity:

In[3]:= FullSimplify[{1, F1[k]/F0[k], F2[k]/F0[k]}]

$$\text{Out}[3] = \left\{ 1, -\frac{(1+k+p)(1+2\nu)}{(-1+k-p)(1+k+2\nu)}, \frac{n(1+k+p)(k+2\nu)}{2(k-n)(-1+k-p)\nu} \right\}$$

In[4]:= Gosper[F0[k], {k, 0, N},

$$\text{Parameterized} \rightarrow \left\{ 1, -\frac{(1+k+p)(1+2\nu)}{(-1+k-p)(1+k+2\nu)}, \frac{n(1+k+p)(k+2\nu)}{2(k-p)(-1+k-p)\nu} \right\}]$$

If 'N' is a natural number, then:

$$\begin{aligned} \text{Out}[4] = & \left\{ \sum_{k=0}^N 4(1+p)\nu(n+\nu)(1+2\nu)F_0[k] - (1+2n+p)(n+2\nu)(1+p+2\nu) \right. \\ & (2+p+2\nu)F_1[k] + 2n\nu(1+2\nu)(1+2n+p+4\nu)F_2[k] == \\ & - ((1+N+p)(1+2\nu)(2n+4n^2+nN+2n^2N+3np+2n^2p+nNp+ \\ & n^2p^2+4\nu+8n\nu+8n^2\nu+2N\nu+6p\nu+8np\nu+2Np\nu+ \\ & 2p^2\nu+8\nu^2+8n\nu^2+8p\nu^2) \\ & \left. \text{Pochhammer}[1-n, N] \text{Pochhammer}[-p, N] \text{Pochhammer}[1+p, N]) / \right. \\ & \left. ((1+N+2\nu)N! \text{Pochhammer}[1, N] \text{Pochhammer}[1+2\nu, N]) \right\} \end{aligned}$$

For $N \rightarrow \infty$ this gives the desired relation because the right hand side is 0 when $N > p$.

The computerized proofs of (5.2)–(5.4) are similar and the corresponding *Mathematica* notebooks are available on the article's website.

6. VIRIAL RECURRENCE RELATIONS

A general procedure of verification of the linear relations between the relativistic integrals can be formulated as follows. Start from the hypergeometric series representations for the integrals involved into the identity/relation in question, and find all linear dependencies between the corresponding hypergeometric series using the package **zb.m**. Substitute the integrals into the desired identity, eliminate the linear dependent sums/vectors from this equation, and then simplify the coefficients in front of the rest of the series to zero with the help of the standard identities among the quantum numbers of the relativistic Coulomb problem.

One can easily see that the linear relation (2.11) is equivalent to (5.4), and that (2.12) follows from (2.11) and (2.13). To illustrate our strategy, we derive (2.13) directly from the hypergeometric representations for the relativistic Coulomb integrals (2.8)–(2.10). To this end, we input the hypergeometric summands involved in the relations (2.8)–(2.10) and (2.13):

In[1]:= <<zb.m

Fast Zeilberger Package by Peter Paule and Markus Schorn (enhanced by Axel Riese)
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$$\begin{aligned}
\text{In}[2] := (\mathbf{a}_-)_k &:= \text{Pochhammer}[\mathbf{a}, k]; & \mathbf{F0}[k_-] &:= \frac{(1-n)_k (-p)_k (p+1)_k}{(2-\nu+1)_k (2)_k k!}; \\
\mathbf{F1}[k_-] &:= \frac{(1-n)_k (-p)_k (p+1)_k}{(2-\nu+1)_k (1)_k k!}; & \mathbf{F2}[k_-] &:= \frac{(-n)_k (-p)_k (p+1)_k}{(2-\nu+1)_k (1)_k k!}; \\
\mathbf{F3}[k_-] &:= \frac{(1-n)_k (-p-1)_k (p+2)_k}{(2-\nu+1)_k (1)_k k!}; & \mathbf{F4}[k_-] &:= \frac{(-n)_k (-p-1)_k (p+2)_k}{(2-\nu+1)_k (1)_k k!};
\end{aligned}$$

$$\text{In}[3] := \text{FullSimplify}[\{1, \mathbf{F1}[k]/\mathbf{F0}[k], \mathbf{F2}[k]/\mathbf{F0}[k], \mathbf{F3}[k]/\mathbf{F0}[k], \mathbf{F4}[k]/\mathbf{F0}[k]\}]$$

$$\text{Out}[3] = \left\{1, 1+k, -\frac{(1+k)n}{k-n}, 1+k+\frac{2k(1+k)}{1-k+p}, \frac{(1+k)n(1+k+p)}{(k-n)(-1+k-p)}\right\}$$

$$\begin{aligned}
\text{In}[4] := \text{Gosper}[\mathbf{F0}[k], \{k, 0, N\}, \text{Parameterized} \rightarrow \{1, 1+k, -\frac{(1+k)n}{k-n}, 1+k+\frac{2k(1+k)}{1-k+p}, \\
\frac{(1+k)n(1+k+p)}{(k-n)(-1+k-p)}\}]
\end{aligned}$$

If 'N' is a natural number, then:

$$\begin{aligned}
\text{Out}[4] = & \left\{ \sum_{k=0}^N -n \mathbf{F1}[k] + (1+n+p) \mathbf{F2}[k] - n \mathbf{F3}[k] + (-1+n-p) \mathbf{F4}[k] == 0, \right. \\
& \sum_{k=0}^N 2n p \mathbf{F0}[k] + (1+2n+p+2\nu) \mathbf{F2}[k] + (-1-p-2\nu) \mathbf{F4}[k] == \\
& \frac{2n(1+N+p) \text{Pochhammer}[1-n, N] \text{Pochhammer}[-p, N] \text{Pochhammer}[1+p, N]}{N! \text{Pochhammer}[2, N] \text{Pochhammer}[1+2\nu, N]}, \\
& \sum_{k=0}^N -2n(n+2\nu) \mathbf{F1}[k] + (1+2n+2n^2+2p+2np+p^2+2\nu+ \\
& 4n\nu+2p\nu) \mathbf{F2}[k] - (1+p)(1+p+2\nu) \mathbf{F4}[k] == \\
& \left. \frac{2n(1+N)(1+N+p) \text{Pochhammer}[1-n, N] \text{Pochhammer}[-p, N] \text{Pochhammer}[1+p, N]}{N! \text{Pochhammer}[2, N] \text{Pochhammer}[1+2\nu, N]} \right\}
\end{aligned}$$

Notice that for $N \rightarrow \infty$ all the right hand sides vanish because they are 0 when $N > p$.

Summarizing, the package has found the following three linear relations:

$$n(X+U) - (1+n+p)Y + (1-n+p)V = 0, \quad (6.1)$$

$$2npZ + (1+2n+p+2\nu)Y - (1+p+2\nu)V = 0, \quad (6.2)$$

$$\begin{aligned}
2n(n+2\nu)X + (1+p)(1+p+2\nu)V \\
= [(n+1)^2 + 2p + (n+p)^2 + 2(2n+p+1)\nu]Y
\end{aligned} \quad (6.3)$$

for the following five linear dependent vectors

$$\begin{aligned} X &:= {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right), & Y &:= {}_3F_2 \left(\begin{matrix} -n, -p, p+1 \\ 2\nu+1, 1 \end{matrix} \right), \\ Z &:= {}_3F_2 \left(\begin{matrix} 1-n, -p, p+1 \\ 2\nu+1, 2 \end{matrix} \right), & U &:= {}_3F_2 \left(\begin{matrix} 1-n, -p-1, p+2 \\ 2\nu+1, 1 \end{matrix} \right), \\ V &:= {}_3F_2 \left(\begin{matrix} -n, -p-1, p+2 \\ 2\nu+1, 1 \end{matrix} \right). \end{aligned}$$

We choose to present everything in terms of Y and V :

```
In[5] := Lin1 = n*(X + U) - (1 + n + p)*Y + (1 - n + p)*V ;
        Lin2 = (2 n p)*Z + (1 + 2 n + p + 2 ν)*Y - (1 + p + 2 ν)*V ;
        Lin3 = -2 n (n + 2 ν)*X +
                (1 + 2 n + 2 n2 + 2 p + 2 n p + p2 + 2 ν + 4 n ν + 2 p ν)*Y -
                (1 + p) (1 + p + 2 ν)*V ;
        Solve[Lin1==0 && Lin2==0 && Lin3==0, {X, U, Z}];
        FullSimplify[%]
```

$$\begin{aligned} \text{Out}[5] = \{ \{ X \rightarrow \frac{-(1+p) V (1+p+2 \nu) + Y (2 n^2 + 2 n (1+p+2 \nu) + (1+p) (1+p+2 \nu))}{2 n (n+2 \nu)}, \\ U \rightarrow \frac{V (2 n^2 - 2 n (1+p-2 \nu) + (1+p) (1+p-2 \nu)) - (1+p) Y (1+p-2 \nu)}{2 n (n+2 \nu)}, \\ Z \rightarrow \frac{V (1+p+2 \nu) - Y (1+2 n+p+2 \nu)}{2 n p} \} \} \end{aligned}$$

Introducing the Coulomb integrals,

```
In[6] := Ap[X, Y, Z] := (2 μ (2 a β)^(p) (Gamma[2 ν + 1])/(Gamma[2 ν + p + 1]))^(-1)*
        ((μ + a κ)*X + (μ - a κ)*Y + 2 p ε a n*Z) ;
        Bp[X, Y, Z] := (2 μ (2 a β)^(p) (Gamma[2 ν + 1])/(Gamma[2 ν + p + 1]))^(-1)*
        (ε (μ + a κ)*X + ε (μ - a κ)*Y + 2 p a n*Z) ;
        Cplus1[U, V] := (4 μ (2 a β)^(p+1) (Gamma[2 ν + 1])/
        (Gamma[2 ν + p + 2]))^(-1)*(a (μ + a κ)*U + a (μ - a κ)*V) ;
```

we express the desired relation in terms of X, \dots, V :

```
In[7] := (2 κ)*Bp[X, Y, Z] - (p+1)*Ap[X, Y, Z] - (4 β)*Cplus1[U, V];
        % /. Gamma[2 + p + 2 ν] -> (1 + p + 2 ν)*Gamma[1 + p + 2 ν];
        FullSimplify[%]
```

$$\begin{aligned} \text{Out}[7] = & -\frac{1}{\mu \text{Gamma}[1+2 \nu]} 2^{-1-p} (a \beta)^{-p} \\ & (\mu ((X+Y) (1+p-2 \varepsilon \kappa) + U (1+p+2 \nu) - V (1+p+2 \nu)) + \\ & a (2 n p Z (\varepsilon + p \varepsilon - 2 \kappa) + \kappa ((X-Y) (1+p-2 \varepsilon \kappa) + \\ & U (1+p+2 \nu) + V (1+p+2 \nu)))) \text{Gamma}[1+p+2 \nu] \end{aligned}$$

Next we rewrite the relevant part into a linear combination of X, \dots, V :

$$\begin{aligned} \text{In}[8] := \text{ZERO} = & (\mu ((X+Y) (1+p-2 \varepsilon \kappa) + U (1+p+2 \nu) - V (1+p+2 \nu)) + \\ & a (2 n p Z (\varepsilon + p \varepsilon - 2 \kappa) + \\ & \kappa ((X-Y) (1+p-2 \varepsilon \kappa) + U (1+p+2 \nu) + V (1+p+2 \nu)))) ; \\ \text{Collect}[\text{ZERO}, \{X, Y, Z, U, V\}] ; \\ \text{FullSimplify}[\%] \end{aligned}$$

$$\begin{aligned} \text{Out}[8] = & 2 a n p Z (\varepsilon + p \varepsilon - 2 \kappa) + Y (1+p-2 \varepsilon \kappa) (-a \kappa + \mu) + \\ & X (1+p-2 \varepsilon \kappa) (a \kappa + \mu) + V (a \kappa - \mu) (1+p+2 \nu) + U (a \kappa + \mu) (1+p+2 \nu) \end{aligned}$$

Eliminating X, U and Z ,

$$\begin{aligned} \text{In}[9] := \% /. \{ & X \rightarrow \frac{-(1+p) V (1+p+2 \nu) + Y (2 n^2 + 2 n (1+p+2 \nu) + (1+p) (1+p+2 \nu))}{2 n (n+2 \nu)}, \\ & U \rightarrow \frac{V (2 n^2 - 2 n (1+p-2 \nu) + (1+p) (1+p-2 \nu)) - (1+p) Y (1+p-2 \nu)}{2 n (n+2 \nu)}, \\ & Z \rightarrow \frac{V (1+p+2 \nu) - Y (1+2 n+p+2 \nu)}{2 n p} \} ; \\ \text{FullSimplify}[\%] ; \\ \text{Collect}[\%, \{Y, V\}] ; \\ \text{FullSimplify}[\%] \end{aligned}$$

$$\begin{aligned} \text{Out}[9] = & \frac{(1+p) V (1+p+2 \nu) (-\mu (n-\varepsilon \kappa + \nu) + a (n^2 \varepsilon - n \kappa + \varepsilon \kappa^2 + 2 n \varepsilon \nu - \kappa \nu))}{n (n+2 \nu)} + \\ & Y \left((1+p-2 \varepsilon \kappa) (-a \kappa + \mu) - \frac{(1+p) (a \kappa + \mu) (1+p-2 \nu) (1+p+2 \nu)}{2 n (n+2 \nu)} - \right. \\ & a (\varepsilon + p \varepsilon - 2 \kappa) (1+2 n+p+2 \nu) + \\ & \left. \frac{(1+p-2 \varepsilon \kappa) (a \kappa + \mu) (2 n^2 + 2 n (1+p+2 \nu) + (1+p) (1+p+2 \nu))}{2 n (n+2 \nu)} \right) \end{aligned}$$

Finally, we simplify the coefficients of V and Y :

```
In[10]:= ZeroV = - μ (n - ε κ + ν) + a (n2 ε - n κ + ε κ2 + 2 n ε ν - κ ν) ;
ZeroY = 2 n (1 + p - 2 ε κ) (-a κ + μ) (n + 2 ν) -
(1 + p) (a κ + μ) (1 + p - 2 ν) (1 + p + 2 ν) -
2 a n (ε + p ε - 2 κ) (n + 2 ν) (1 + 2 n + p + 2 ν) +
(1 + p - 2 ε κ) (a κ + μ) (2 n2 + 2 n (1 + p + 2 ν) + (1 + p) (1 + p + 2 ν)) ;
{ZeroV, ZeroY} ;
FullSimplify[%] ;
% /. n -> (ε μ - a ν)/a ;
FullSimplify[%] ;
% /. ε2 -> 1 - a2 ;
FullSimplify[%] ;
% /. κ2 -> ν2 + μ2
```

```
Out[10]= {0, 0}
```

which is the name of the game.

Computerized proofs of (2.14) and some of its extensions work the same; they are available on the article's website.

In a similar fashion, seeking for a more general linear combination of the corresponding integrals, with the **zb.m** package one can derive the following two-parameter relation:

$$[D(p+1) - C(2\kappa + \varepsilon(p+1))]A_p - [2D\kappa - C(2\varepsilon\kappa + p+1)]B_p + 4\mu C C_p + 4\beta D C_{p+1} = 0, \quad (6.4)$$

where C and D are two arbitrary constants. The virial relations (2.11)–(2.13) are its special cases.

We would like to point out the following relation:

$$(p+1)(2\kappa C_p - \mu A_p) = \beta(p+2)(\varepsilon A_{p+1} - B_{p+1}), \quad (6.5)$$

as another simple example.

Note. This relation is a linear combination of (2.12)–(2.14); see [1].

7. CONCLUSION

The relativistic Coulomb integrals (2.4)–(2.6) were recently evaluated in a hypergeometric form [36]. The corresponding system of the first order difference equations (2.15)–(2.16) has been solved in [38] in terms of linear combinations of the dual Hahn polynomials thus providing an independent proof. Here, with the help of the Fast Zeilberger Package **zb.m** we give a direct derivation of these results.

One of the goals of this article is to demonstrate the power of symbolic computation for the study of relativistic Coulomb integrals. Namely, computer algebra methods related to Zeilberger's holonomic systems approach allow not only to verify some already known complicated relations,

but also to derive new ones without making enormously time-consuming calculations by hands or with ad hoc usage of computer algebra procedures.

In a sequel to this article we are planning to investigate the computer-assisted derivation of recurrences, e.g. the “birthday recurrences” from Section 4, by taking as a starting point the original definition of the Coulomb integrals (2.4)–(2.6). To this end, we will use Koutschan’s package `HolonomicFunctions` [16]. This package, written in *Mathematica*, implements further ideas related to Zeilberger’s holonomic systems paradigm [41]; for instance, it includes implementations of (variations of) Z’s “slow algorithm”, and algorithms by F. Chyzak (and B. Salvy), and N. Takayama. In this context we will have to exploit closure properties of classes of special (resp. holonomic) sequences and functions; an introduction to computer algebra methods for the univariate case can be found in [15].

Moreover, the `zb.m` package strongly suggests that there are, in fact, four linearly independent virial recurrence relations, see more details on the article’s website, but only three of them (e. g., (2.12)–(2.14)) are available in the literature. Another next challenge is to study the off-diagonal matrix elements that are important in applications [23], [24], [25], [29], [30], and [33].

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